Development of Highly Selective Oxidation Catalysts by Atomic Layer Deposition

New Synthesis Techniques Promise More Effective Catalysts and Drastic Energy Savings

Alkenes such as ethylene, propylene, and butadiene are feedstocks in the production in many plastics, construction materials, insulators, household items, and textiles. Providing an adequate supply of these short-chain alkenes (C2, C3, C4) is vital to keeping up with ever-increasing manufacturing demands. Currently, a wide variety of hydrocarbons are converted to the alkenes by cracking, a process demanding extremely high energy and capital investments. Oxidative dehydrogenation of short-chain alkanes would represent an energy-savings alternative to cracking but is not a viable choice for two reasons. The first reason is that catalysts do not yield enough quality product at high rates. The second reason is that the industry already has costly cracking furnaces in place and would need considerable economic motivation to switch. A catalyst that significantly increases percentage yields and overall throughput of alkenes would make oxidative dehydrogenation a more realistic option to cracking.

This project aims to use Atomic Layer Deposition (ALD) to improve catalysts involved in oxidative dehydrogenation, converting alkanes to alkenes. ALD has been proven to work on catalysts converting cyclohexane to cyclohexene, and, in this project, researchers hope to extend this capability to the oxidative dehydrogenation of short-chain alkanes. Researchers will apply already established principles to produce homogenous and more effective catalysts and to enhance overall understanding of oxidative dehydrogenation. Successful results will provide an energy-efficient and economically feasible alternative for alkene production.

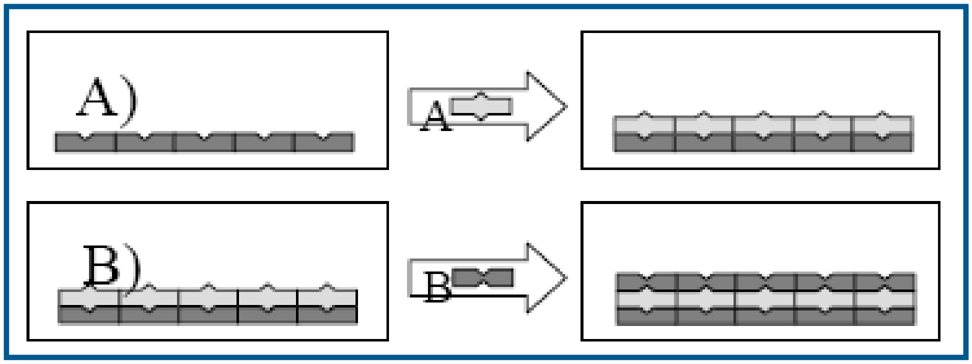
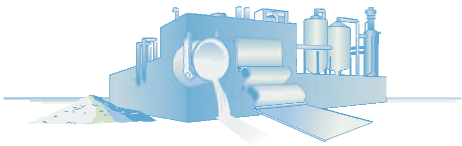


Illustration of the ALD process. Reaction A deposits a monolayer of A species with atomic layer precision on the substrate. This becomes the starting surface for Reaction B, which deposits monolayer B in the same fashion. The process repeats itself (ABAB…) until a catalyst layer with the desired thickness is achieved.



Benefits for Our Industry and Our Nation

More effective catalysts for oxidation dehydrogenation of alkanes could enable higher specific conversion rates and result in drastic energy savings. Improving catalysts that convert alkanes to alkenes promises to save up to 25 trillion Btu per year by 2020.

Applications in Our Nation's Industry

The results of this research will find immediate application in the conversion of short-chain alkanes to alkenes. Industries will experience higher yields of ethylene, propylene, and butadiene at lower energy costs for economic savings.

Project Description

The goal of this project is to use ALD to construct nanostructured catalysts to improve the effectiveness of oxidative dehydrogenation of alkanes. This would provide an economic and energy-efficient option to the cracking of hydrocarbons.

Barriers

Major barriers to be overcome include:

- Existing methods of industrial catalyst production provide poor control over the uniformity and dispersion of the catalyst.
- Methods must be developed to synthesize certain oxide materials and combinations of materials using ALD techniques.
- Maintaining monolayer control over composition and thickness of catalyst layers in large quantities of nanoporous catalyst support materials.
- Achieving optimal composition of ALD catalyst to obtain greatest conversion and highest selectivity to the alkene product.
- Scale-up of ALD processes for industrial catalyst fabrication have never before been demonstrated
- Extension of ALD methods for catalyst manufacture from conventional powder substrates to nanoporous membrane substrates.

Pathways

The objectives of this project will be achieved through (1) using ALD techniques to produce novel catalytic materials on conventional powder substrates; (2) determining the optimal catalyst composition to provide superior performance compared to conventional catalysts; (3) applying these catalytic films to oxidative dehydrogenation reactions on short-chain alkanes; (4) scaling up production catalyst manufacturing to larger quantities for industrial applications; (5) application ALD catalysts to nanoporous catalytic membranes for use in single-pass catalytic reactors.

Progress and Milestones

- Develop ALD processes for vanadium oxide, niobium oxide, "transition metal y" oxide, and silica for deposition on flat surfaces (completed)
- Synthesize, characterize, and test ALD coated silica powder catalysts for the oxidative dehydrogenation of short chain alkanes (completed)
- Synthesize, characterize, and test ALD coated nanoporous anodic alumina membranes for the oxidative dehydrogenation of short chain alkanes
- Scale-up and demonstrate a pilot-scale of the technology to coat catalytic powders using ALD
- Evaluate new process economics

Commercialization

The project has various partners that will participate in developing and commercializing the technology. Argonne National Laboratory will focus on catalyst preparation and Ineos Technologies, LLC (formerly BP Amoco Chemicals) and Northwestern University will focus on industrial characterization and catalyst testing. Together these partners include several chemists with expertise in catalyst preparation and screening, several analytical chemists for catalyst characterization, and a quantum chemist for molecular modeling. This multi-disciplinary team has an established infrastructure to not only perform the project tasks but also to commercialize promising new catalysts.

Project Partners

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A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy
Bringing you a prosperous future where energy is clean, abundant, reliable and affordable

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